

# Variational calculations of dispersion coefficients for interactions between H, He, and Li atoms

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## Abstract

The dispersion coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for the interactions between H, He, and Li are calculated using variational wave functions in Hylleraas basis sets with multiple exponential scale factors. With these highly correlated wave functions, significant improvements are made upon previous calculations and our results provide definitive values for these coefficients.

## I. INTRODUCTION

At large separations  $R$ , the interaction potential between two neutral atoms can be expressed in terms of inverse powers of  $R$ , with the leading term  $R^{-6}$  [1,2]. The nature of the long-range interaction can be described by the mutual perturbations of instantaneous multipoles of individual atoms. The coefficient of the  $R^{-6}$  term comes from an instantaneous dipole-dipole interaction and the coefficient of the  $R^{-8}$  term from an instantaneous dipole-quadrupole interaction.

The precise evaluation of the dispersion coefficients between atoms is computationally challenging, because it requires a summation over all intermediate states, including the continuum. In actual calculations, it is therefore essential to have an adequate representation of the whole spectrum of the Hamiltonian. For atomic systems with more than one electron the central problem is the inclusion of electron-electron correlations.

Recently, significant progress [3,4] has been made in variational calculations for the helium and lithium atoms using double and multiple basis sets in Hylleraas coordinates. The nonrelativistic energies for helium have been obtained to better than one part in  $10^{16}$  for the entire singly-excited spectrum, whereas the nonrelativistic energies for the low-lying states of lithium are accurate to a few parts in  $10^{11}$  to  $10^{12}$  [5]. We have also performed a high precision calculation for the lithium  $2^2S \rightarrow 2^2P$  oscillator strength [6] which has been a subject of controversy for many years. Although there have been many calculations for the dispersion coefficients between H, He, and Li (see for example, [2,7–11]), the results involving Li vary over a considerable range.

Due to the recent progress of ultracold collisions in both theory and experiment [12], precise forms of long-range interaction potentials between various atoms become very important. The purpose of this paper is to present the results of variational calculations in Hylleraas basis sets using multiple nonlinear parameters. The use of our highly correlated wave functions will improve upon previous calculations and provide more definitive values for the dispersion coefficients.

The theory of long-range forces is outlined in Sec. II. The structures of the basis sets for one, two, and three electron atomic systems are presented in Sec. III. Our final results are tabulated and comparisons are made with the various previous calculations. In the appendix, a derivation is given of the dispersion coefficients for the Li(*S*)-Li(*P*) system.

## II. FORMULATION

### A. Ground state dispersion coefficients

In this section, we concentrate on interactions between atoms in their ground states. Using second-order perturbation theory, the long-range part of interaction between two atoms a and b in their ground states can be expanded in terms of a series of inverse powers of the separation  $R$  [1,2]

$$V_{ab} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} \cdots, \quad (1)$$

where the coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  are

$$C_6 = \frac{3}{\pi} G_{ab}(1, 1), \quad (2)$$

$$C_8 = \frac{15}{2\pi} G_{ab}(1, 2) + \frac{15}{2\pi} G_{ab}(2, 1), \quad (3)$$

$$C_{10} = \frac{14}{\pi} G_{ab}(1, 3) + \frac{14}{\pi} G_{ab}(3, 1) + \frac{35}{\pi} G_{ab}(2, 2), \quad (4)$$

where

$$G_{ab}(l_a, l_b) = \int_0^\infty \alpha_{l_a}^a(i\omega) \alpha_{l_b}^b(i\omega) d\omega. \quad (5)$$

In (5),  $\alpha_{l_a}^a(i\omega)$  is the dynamic  $2^{l_a}$  polarizability for atom a at imaginary frequency  $i\omega$ . The dynamic polarizability can be expressed in terms of a sum over all intermediate states, including the continuum (in atomic units throughout):

$$\alpha_l(\omega) = \sum_n \frac{f_{n0}^{(l)}}{E_{n0}^2 - \omega^2} \quad (6)$$

with the  $2^l$ -pole oscillator strength  $f_{n0}^{(l)}$  being defined by

$$f_{n0}^{(l)} = \frac{8\pi}{2l+1} E_{n0} |\langle \Psi_0 | \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) | \Psi_n \rangle|^2, \quad (7)$$

where  $E_{n0} = E_n - E_0$ , the sum  $i$  runs over all the electrons in the atom,  $\Psi_0$  is the ground state wave function,  $E_0$  is the corresponding ground state energy, and  $\Psi_n$  is the  $n$ th intermediate eigenfunction with the associated eigenvalue  $E_n$ . An oscillator strength  $\bar{f}_{n0}^{(l)}$  which is independent of magnetic quantum number  $m$  is obtained by averaging over the initial state orientation degeneracy and summing over the final state degeneracy. It is convenient to introduce reduced matrix elements through the Wigner-Eckart theorem [13]

$$\langle \gamma' L' M' | \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) | \gamma L M \rangle = (-1)^{L'-M'} \begin{pmatrix} L' & l & L \\ -M' & m & M \end{pmatrix} \langle \gamma' L' || \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) || \gamma L \rangle. \quad (8)$$

With the aid of a sum rule for the  $3-j$  symbols, the oscillator strength can be written

$$\bar{f}_{n0}^{(l)} = \frac{8\pi}{(2l+1)^2(2L_0+1)} E_{n0} |\langle \Psi_0 || \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) || \Psi_n \rangle|^2, \quad (9)$$

where  $L_0$  is the total angular momentum for the initial state.

Using the identity

$$\frac{2}{\pi} \int_0^\infty \frac{d\omega}{(a^2 + \omega^2)(b^2 + \omega^2)} = \frac{1}{ab(a+b)}, \quad a, b > 0 \quad (10)$$

we can recast Eq. (5) into the equivalent form

$$G_{ab}(l_a, l_b) = \frac{\pi}{2} \sum_{nn'} \frac{f_{n0}^{(l_a)} f_{n'0}^{(l_b)}}{E_{n0}^a E_{n'0}^b (E_{n0}^a + E_{n'0}^b)}, \quad (11)$$

where  $E_{n0}^i = E_n^i - E_0^i$  is the excitation energy for atom  $i$  and is always positive for the atoms in the ground state. The procedure for evaluating  $G_{ab}(l_a, l_b)$  is to diagonalize Hamiltonian in a basis set and sum over all intermediate states directly according to (11), and a convergence study can be done by increasing the size of basis set progressively.

The long-range part of the interaction between three ground state atoms is not exactly equal to the interaction energies taken in pairs. There is a non-additive term which comes from the third order perturbation. The leading terms in the expression for the dispersion energy of the three-atom system are [1,2]

$$V_{\text{abc}} = -\frac{C_6^{\text{ab}}}{r_{\text{ab}}^6} - \frac{C_6^{\text{bc}}}{r_{\text{bc}}^6} - \frac{C_6^{\text{ca}}}{r_{\text{ca}}^6} - \frac{\nu_{\text{abc}}(3 \cos \theta_{\text{a}} \cos \theta_{\text{b}} \cos \theta_{\text{c}} + 1)}{(r_{\text{ab}} r_{\text{bc}} r_{\text{ca}})^3}, \quad (12)$$

where  $\theta_{\text{a}}$ ,  $\theta_{\text{b}}$ , and  $\theta_{\text{c}}$  are the internal angles of the triangle formed by  $r_{\text{ab}}$ ,  $r_{\text{bc}}$  and  $r_{\text{ca}}$ , and  $\nu_{\text{abc}}$  is the triple-dipole constant defined by

$$\nu_{\text{abc}} = \frac{3}{\pi} \int_0^\infty \alpha_1^{\text{a}}(i\omega) \alpha_1^{\text{b}}(i\omega) \alpha_1^{\text{c}}(i\omega) d\omega. \quad (13)$$

## B. Excited state dispersion coefficients

For two like atoms which are not both in their ground states, the perturbation theory for calculating the dispersion coefficients was given by Marinescu and Dalgarno [10]. They worked out all the details for evaluating the dispersion coefficients of alkali-metal dimers in different excited states within a one-electron model potential formalism. In this work, we examine the important case when one lithium atom is in the  $2^2S$  ground state and the other lithium atom is in the  $2^2P$  state. A detailed derivation for many-electron systems is given at the Appendix.

The zero-order wave function for the  $\text{Li}(S)\text{-Li}(P)$  system can be written as a symmetrized product of two individual atomic wave functions

$$\Psi^{(0)} = \frac{1}{\sqrt{2}} [\Psi_{\text{a}}(L_1 M_1; \mathbf{r}) \Psi_{\text{b}}(L_2 M_2; \rho) + \beta \Psi_{\text{a}}(L_1 M_1; \rho) \Psi_{\text{b}}(L_2 M_2; \mathbf{r})], \quad (14)$$

where  $\mathbf{r}$  and  $\rho$  represent all the internal coordinates for the two atoms respectively,  $L_1$  and  $L_2$  are their total orbital angular momenta,  $M_1$  and  $M_2$  are the associated magnetic quantum numbers, and  $\beta = \pm 1$  describes the symmetry due to Pauli exclusion principle. Following [10], first-order perturbation theory yields the interaction energy

$$V^{(1)}(L_2 M_2; \beta) = -\frac{C_{2L_2+1}^{M_2 \beta}}{R^{2L_2+1}}, \quad (15)$$

where

$$C_{2L_2+1}^{M_2 \beta} = \beta (-1)^{1+L_2+M_2} \frac{4\pi}{(2L_2+1)^2} \binom{2L_2}{L_2+M_2} |\langle \Psi_{\text{a}}(0; \mathbf{r}) | \sum_i r_i^{L_2} Y_{L_2}(\hat{\mathbf{r}}_i) | \Psi_{\text{b}}(L_2; \mathbf{r}) \rangle|^2. \quad (16)$$

The first-order energy correction is proportional to  $\beta$ . Therefore, for two unlike atoms ( $\beta = 0$ ) in the asymptotic region where overlap between two atoms can be neglected, there is no first-order correction to the interaction. For two like atoms, however, there is a first-order correction to the interaction energy as long as two atoms are in different angular momentum states. For the Li(*S*)-Li(*P*) system, the interaction is proportional to  $R^{-3}$ . The interaction between two ground state atoms is always attractive (see (1)) but the interaction between two like atoms in different angular momentum states is equally likely to be attractive and repulsive.

The leading energy correction obtained from the second-order perturbation theory for the Li(*S*)-Li(*P*) system is

$$V^{(2)} = -\frac{C_6^{M_2}}{R^6}, \quad (17)$$

where

$$C_6^{M_2} = \sum_{st} \frac{\Omega_{st}}{E_{st}^{(0)} - E^{(0)}} \quad (18)$$

with

$$\begin{aligned} \Omega_{st} = & |\langle \Psi_a(0; \mathbf{r}) | \sum_i r_i Y_1(\hat{\mathbf{r}}_i) | \chi(1; \mathbf{r}) \rangle|^2 \\ & \times \sum_{\lambda} G(1, 1, 1, \lambda, 1, M_2) |\langle \Psi_b(1; \rho) | \sum_j \rho_j Y_1(\hat{\rho}_j) | \omega(\lambda; \rho) \rangle|^2. \end{aligned} \quad (19)$$

In (18), the summation should exclude one term which gives rise to  $E_{st}^{(0)} = E^{(0)}$ . Note that  $C_6^{M_2}$  is independent of  $\beta$ . The values of  $G$  are listed in Table I.

It should be noted that the terms with  $\lambda = 1$  in (19), which corresponds to transitions between even parity states  $P^e$  and odd parity state  $P^o$ , are missing in one-electron model potential methods [10]. The dominant contribution comes from the radiative transition between the lowest doubly excited doublet state  $1s2p2p^2P^e$ , which is stable against autoionization [14], to the singly excited doublet state  $1s^22p^2P^o$ . The contribution of the  $\lambda = 1$  term to  $C_6^{M_2}$  is 0.980 82(5) for  $M_2 = \pm 1$ , and 0.392 32(2) for  $M_2 = 0$ .

### III. CALCULATIONS AND RESULTS

For the hydrogen atom, the following Sturmian basis set [15] is used to diagonalize the Hamiltonian:

$$\{r^l e^{-\beta r/2} L_n^{(2l+2)}(\beta r)\}, \quad (20)$$

where  $L_n^{(2l+2)}(\beta r)$  is the generalized Laguerre polynomial and the parameter  $\beta$  is chosen to be  $\beta = 2/(l+1)$ . This basis set has proven to be numerically stable as the size of basis set is enlarged.

For the helium atom, the basis set is constructed using Hylleraas coordinates [16]

$$\{\chi_{ijk} = r_1^i r_2^j r_{12}^k e^{-\alpha r_1 - \beta r_2}\}, \quad (21)$$

and the wave functions are expanded from doubled basis sets. The explicit form for the wave function is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{ijk} [a_{ijk}^{(1)} \chi_{ijk}(\alpha_1, \beta_1) + a_{ijk}^{(2)} \chi_{ijk}(\alpha_2, \beta_2)] \pm \text{exchange}, \quad (22)$$

and  $i + j + k \leq \Omega$ . A complete optimization is then performed with respect to the two sets of nonlinear parameters  $\alpha_1, \beta_1$ , and  $\alpha_2, \beta_2$ . The screened hydrogenic wave function is also included explicitly in the basis set. These techniques yield much improved convergence relative to single basis set calculations.

For the lithium atom, the basis set is also constructed in Hylleraas coordinates [4]

$$\{\phi_{t,\mu_t}(\alpha_t, \beta_t, \gamma_t) = r_1^{j_1} r_2^{j_2} r_3^{j_3} r_{12}^{j_{12}} r_{23}^{j_{23}} r_{31}^{j_{31}} e^{-\alpha_t r_1 - \beta_t r_2 - \gamma_t r_3}\}, \quad (23)$$

where  $\mu_t$  denotes a sextuple of integer powers  $j_1, j_2, j_3, j_{12}, j_{23}$ , and  $j_{31}$ , index  $t$  labels different sets of nonlinear parameters  $\alpha_t, \beta_t$  and  $\gamma_t$ . Except for some truncations, all terms are included such that

$$j_1 + j_2 + j_3 + j_{12} + j_{23} + j_{31} \leq \Omega. \quad (24)$$

The wave function is expanded from the multiple basis sets

$$\begin{aligned}\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = & \mathcal{A} \sum_t \sum_{\mu_t} a_{t,\mu_t} \phi_{t,\mu_t}(\alpha_t, \beta_t, \gamma_t) \\ & \times (\text{angular function})(\text{spin function}).\end{aligned}\quad (25)$$

A similar optimization is also performed with respect to all the nonlinear parameters.

Table II contains the values of the static polarizabilities  $\alpha_1(0)$ ,  $\alpha_2(0)$ , and  $\alpha_3(0)$  for H, He, and Li in their ground states. Tables III and IV present the comparison with selected previous calculations for He and Li. Using the Sturmian basis sets containing up to 70 terms yields the well-known exact results for the H atom. For He, the largest size of basis set for the ground state is 504. For the intermediate states, the largest sizes of basis sets are 728, 733, and 792 respectively for the  $P$ ,  $D$ , and  $F$  symmetries. Table III shows that our value for  $\alpha_1(0)$  is in perfect agreement with the best previous results of Bishop and Pipin [7] and Jamieson *et al.* [9] within the first 7 digits. However, our value of  $\alpha_1(0)$ , as well as  $\alpha_2(0)$  and  $\alpha_3(0)$ , has converged to several more significant figures, as indicated by the extrapolation uncertainty in parentheses. For Li, with the fixed size of basis set 919 for the ground state, Table V contains the convergence studies of  $\alpha_1(0)$  in both length and velocity forms, as the number of terms for the intermediate  $P$  symmetry is progressively increased. As a further numerical check, we calculated  $\alpha_1(0)$  for the Li atom by solving an inhomogeneous equation, using the Dalgarno-Lewis method [21] as follows:

$$\alpha_l(0) = -\frac{8\pi}{2l+1} \langle \Psi(2^2S) | \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) | \Psi_1 \rangle, \quad (26)$$

where  $\Psi_1$  satisfies the inhomogeneous equation

$$(H_0 - E_0)\Psi_1 + \left(\sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) - E_1\right)\Psi(2^2S) = 0. \quad (27)$$

In the above equation,  $H_0$  is the unperturbed Li Hamiltonian,  $E_0$  is the Li ground state energy, and

$$E_1 = \langle \Psi(2^2S) | \sum_i r_i^l Y_{lm}(\hat{\mathbf{r}}_i) | \Psi(2^2S) \rangle. \quad (28)$$

Eq. (27) is solved variationally by expanding  $\Psi_1$  in terms of a Hylleraas basis set. The two procedures are equivalent. Using basis sets up to 2136,  $\alpha_1(0)$  converges monotonically



to 164.1098. Based on these convergence studies, our final extrapolated value of  $\alpha_1(0)$  is 164.111(2). We have also done similar convergence studies for  $\alpha_2(0)$  and  $\alpha_3(0)$ . Our results for  $\alpha_1(0)$  and  $\alpha_2(0)$  are in good accord with the results of Pipin and Bishop [22]. The model potential results of Marinescu *et al.* [8] agree with the present calculations at the 0.05% and 0.1% levels for  $\alpha_2(0)$  and  $\alpha_3(0)$  respectively.

Table VI shows our values of the two-body dispersion coefficients  $C_6$ ,  $C_8$ , and  $C_{10}$  for the ground state H, He, and Li atoms. For the H-H case, these coefficients can be calculated to arbitrarily high precision. Our value of  $C_6$  is in complete agreement with the value of Margoliash and Meath [36]. Comparisons with the previous calculations for He( $1^1S$ )-He( $1^1S$ ) and Li( $2^2S$ )-Li( $2^2S$ ) are listed in Tables VII and VIII.

For the He-He case, our  $C_6$  and  $C_8$  are in excellent agreement with the results of Bishop and Pipin [7], but more precise by about three orders of magnitude. As for  $C_{10}$ , a small disagreement of about 1 ppm exists. The value of Jamieson *et al.* [9] for  $C_6$  also agrees with our value.

For the Li-Li case, convergence studies for  $C_6$  in both length and velocity forms are listed in Table V. The agreement between the two forms is satisfactory. From Table VIII, it can be seen that the result of Stacey and Dalgarno [41] for  $C_6$  is in close agreement with the present calculation. The model potential results of Marinescu *et al.* [8] for  $C_6$ ,  $C_8$ , and  $C_{10}$  differ from our calculations at the 0.1% to 0.3% level.

Table IX lists the triple-dipole constants  $\nu_{abc}$  for the combinations between three ground state atoms H, He, and Li, together with the previous values of Stacey and Dalgarno [41]. The overall agreement is about 1%.

Finally, Tables X and XI list values of  $C_3$  and  $C_6$  and a comparison with the previous calculations for the interaction between the ground state Li( $2^2S$ ) and the excited Li( $2^2P$ ).  $C_3$ , which is proportional to the square of the resonant dipole matrix element, has recently been calculated to high precision [6]. As for  $C_6$ , our values agree with the model potential calculations of Marinescu and Dalgarno [10] at about the 0.3% level.

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## APPENDIX A:

In the appendix, we discuss the dispersion coefficients for the Li(*S*)-Li(*P*) system. The zero-order wave function for this system can be written as a symmetrized product of two individual atomic wave functions

$$\Psi^{(0)} = \frac{1}{\sqrt{2}} [\Psi_a(L_1 M_1; \mathbf{r}) \Psi_b(L_2 M_2; \rho) + \beta \Psi_a(L_1 M_1; \rho) \Psi_b(L_2 M_2; \mathbf{r})], \quad (\text{A1})$$

where  $\mathbf{r}$  and  $\rho$  represent all the internal coordinates for the two atoms respectively,  $L_1$  and  $L_2$  are their total orbital angular momenta,  $M_1$  and  $M_2$  are the associated magnetic quantum numbers, and  $\beta = \pm 1$  describes the symmetry due to Pauli exclusion principle. Following [10], the interaction potential for two neutral atoms is

$$V = \sum_{l=1}^{\infty} \sum_{L=1}^{\infty} \frac{V_{lL}}{R^{l+L+1}}, \quad (\text{A2})$$

where

$$V_{lL} = (-1)^L 4\pi (l, L)^{-1/2} \sum_{ij} \sum_{\mu} K_{lL}^{\mu} r_i^l \rho_j^L Y_{l\mu}(\hat{\mathbf{r}}_i) Y_{L-\mu}(\hat{\rho}_j). \quad (\text{A3})$$

In the above equation,  $(l, L, \dots) = (2l+1)(2L+1)\dots$ , and

$$K_{lL}^{\mu} = \left[ \binom{l+L}{l+\mu} \binom{l+L}{L+\mu} \right]^{1/2}. \quad (\text{A4})$$

### 1. The first-order energy

The first-order energy is given by

$$V^{(1)} = \frac{1}{2}A_1 + \frac{1}{2}A_2 + \beta A_3 \quad (\text{A5})$$

with

$$A_1 = \langle \Psi_a(L_1 M_1; \mathbf{r}) \Psi_b(L_2 M_2; \rho) | V | \Psi_a(L_1 M_1; \mathbf{r}) \Psi_b(L_2 M_2; \rho) \rangle, \quad (\text{A6})$$

$$A_2 = \langle \Psi_a(L_1 M_1; \rho) \Psi_b(L_2 M_2; \mathbf{r}) | V | \Psi_a(L_1 M_1; \rho) \Psi_b(L_2 M_2; \mathbf{r}) \rangle, \quad (\text{A7})$$

$$A_3 = \langle \Psi_a(L_1 M_1; \mathbf{r}) \Psi_b(L_2 M_2; \rho) | V | \Psi_a(L_1 M_1; \rho) \Psi_b(L_2 M_2; \mathbf{r}) \rangle. \quad (\text{A8})$$

Substituting (A2) into (A6), one has

$$\begin{aligned} A_1 &= \sum_{lL\mu} \frac{(-1)^L 4\pi}{R^{l+L+1}} (l, L)^{-1/2} K_{lL}^\mu \langle \Psi_a(L_1 M_1; \mathbf{r}) | \sum_i r_i^l Y_{l\mu}(\hat{\mathbf{r}}_i) | \Psi_a(L_1 M_1; \mathbf{r}) \rangle \\ &\quad \times \langle \Psi_b(L_2 M_2; \rho) | \sum_j \rho_j^L Y_{L-\mu}(\hat{\rho}_j) | \Psi_b(L_2 M_2; \rho) \rangle. \end{aligned} \quad (\text{A9})$$

From the Wigner-Eckart theorem (8), one has

$$\begin{aligned} &\langle \Psi_a(L_1 M_1; \mathbf{r}) | \sum_i r_i^l Y_{l\mu}(\hat{\mathbf{r}}_i) | \Psi_a(L_1 M_1; \mathbf{r}) \rangle \\ &= (-1)^{L_1-M_1} \begin{pmatrix} L_1 & l & L_1 \\ -M_1 & \mu & M_1 \end{pmatrix} \langle \Psi_a(L_1; \mathbf{r}) | \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) | \Psi_a(L_1; \mathbf{r}) \rangle. \end{aligned} \quad (\text{A10})$$

For  $L_1 = 0$ , the  $3-j$  symbol is zero when  $l \geq 1$ . Thus,  $A_1 = 0$ . Similarly,  $A_2 = 0$ . For  $A_3$ , after using the Wigner-Eckart theorem, we obtain

$$\begin{aligned} A_3 &= \sum_{lL\mu} \frac{(-1)^L 4\pi}{R^{l+L+1}} (l, L)^{-1/2} K_{lL}^\mu \langle \Psi_a(L_1; \mathbf{r}) | \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) | \Psi_b(L_2; \mathbf{r}) \rangle \\ &\quad \times \langle \Psi_b(L_2; \rho) | \sum_j \rho_j^L Y_L(\hat{\rho}_j) | \Psi_a(L_1; \rho) \rangle g, \end{aligned} \quad (\text{A11})$$

where, for  $L_1 = 0$ ,

$$\begin{aligned} g &= (-1)^{L_1-M_1} \begin{pmatrix} L_1 & l & L_2 \\ -M_1 & \mu & M_2 \end{pmatrix} (-1)^{L_2-M_2} \begin{pmatrix} L_2 & L & L_1 \\ -M_2 & -\mu & M_1 \end{pmatrix} \\ &= \frac{(-1)^{L_2-M_2}}{2L_2+1} \delta_{l,L_2} \delta_{L,L_2} \delta_{\mu,-M_2}. \end{aligned} \quad (\text{A12})$$

Since [13]

$$\langle L' || Y_l || L \rangle = (-1)^{L'-L} \langle L || Y_l || L' \rangle, \quad (\text{A13})$$

we finally have

$$V^{(1)}(L_2 M_2; \beta) = -\frac{C_{2L_2+1}^{M_2 \beta}}{R^{2L_2+1}}, \quad (\text{A14})$$

where

$$C_{2L_2+1}^{M_2 \beta} = \beta (-1)^{1+L_2+M_2} \frac{4\pi}{(2L_2+1)^2} \binom{2L_2}{L_2+M_2} |\langle \Psi_a(0; \mathbf{r}) | \sum_i r_i^{L_2} Y_{L_2}(\hat{\mathbf{r}}_i) | \Psi_b(L_2; \mathbf{r}) \rangle|^2. \quad (\text{A15})$$

## 2. The second-order energy

Let the complete set of the system be

$$\{\chi(L_s M_s; \mathbf{r}) \omega(L_t M_t; \rho)\} \quad (\text{A16})$$

with the energy eigenvalue  $E_{st}^{(0)} = E_s^{(0)} + E_t^{(0)}$ . The energy for the unperturbed system is  $E^{(0)} = E_1^{(0)} + E_2^{(0)}$ . According to the second-order perturbation theory, the second-order energy is

$$\begin{aligned} V^{(2)} &= - \sum_{st} \frac{|\langle \Psi^{(0)} | V | \chi(L_s M_s; \mathbf{r}) \omega(L_t M_t; \rho) \rangle|^2}{E_{st}^{(0)} - E^{(0)}} \\ &= - \sum_{st} \frac{T}{E_{st}^{(0)} - E^{(0)}}, \end{aligned} \quad (\text{A17})$$

where  $T$  can be written as

$$T = B_1 + B_2 + \beta B_3 \quad (\text{A18})$$

with

$$B_1 = \frac{1}{2} \sum_{L_s M_s} \sum_{L_t M_t} \langle \Psi_a(L_1 M_1; \mathbf{r}) \Psi_b(L_2 M_2; \rho) | V | \chi(L_s M_s; \mathbf{r}) \omega(L_t M_t; \rho) \rangle^2, \quad (\text{A19})$$

$$B_2 = \frac{1}{2} \sum_{L_s M_s} \sum_{L_t M_t} \langle \Psi_a(L_1 M_1; \rho) \Psi_b(L_2 M_2; \mathbf{r}) | V | \chi(L_s M_s; \mathbf{r}) \omega(L_t M_t; \rho) \rangle^2, \quad (\text{A20})$$

$$\begin{aligned}
B_3 = & \sum_{L_s M_s} \sum_{L_t M_t} \langle \Psi_a(L_1 M_1; \mathbf{r}) \Psi_b(L_2 M_2; \rho) | V | \chi(L_s M_s; \mathbf{r}) \omega(L_t M_t; \rho) \rangle \\
& \times \langle \Psi_a(L_1 M_1; \rho) \Psi_b(L_2 M_2; \mathbf{r}) | V | \chi(L_s M_s; \mathbf{r}) \omega(L_t M_t; \rho) \rangle. \quad (\text{A21})
\end{aligned}$$

After using the Wigner-Eckart theorem, we obtain

$$\begin{aligned}
B_1 = & \frac{1}{2} \sum_{l L \mu} \sum_{l' L' \mu'} \sum_{L_s L_t} \sum_{M_s M_t} \frac{(4\pi)^2}{R^{l+L+l'+L'+2}} (-1)^{L+L'} (l, L, l', L')^{-1/2} K_{lL}^\mu K_{l'L'}^{\mu'} \\
& \times \langle \Psi_a(L_1; \mathbf{r}) | \sum_i r_i^l Y_l(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle \langle \Psi_b(L_2; \rho) | \sum_j \rho_j^L Y_L(\hat{\rho}_j) | \omega(L_t; \rho) \rangle \\
& \times \langle \Psi_a(L_1; \mathbf{r}) | \sum_i r_i^{l'} Y_{l'}(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle \langle \Psi_b(L_2; \rho) | \sum_j \rho_j^{L'} Y_{L'}(\hat{\rho}_j) | \omega(L_t; \rho) \rangle \\
& \times \begin{pmatrix} L_1 & l & L_s \\ -M_1 & \mu & M_s \end{pmatrix} \begin{pmatrix} L_2 & L & L_t \\ -M_2 & -\mu & M_t \end{pmatrix} \begin{pmatrix} L_1 & l' & L_s \\ -M_1 & \mu' & M_s \end{pmatrix} \begin{pmatrix} L_2 & L' & L_t \\ -M_2 & -\mu' & M_t \end{pmatrix}. \quad (\text{A22})
\end{aligned}$$

For  $L_1 = 0$ , the product of four  $3-j$  symbols becomes

$$\delta_{l, L_s} \delta_{l', L_s} \delta_{\mu, -M_s} \delta_{\mu', -M_s} \frac{1}{2L_s + 1} \begin{pmatrix} L_2 & L & L_t \\ -M_2 & M_s & M_t \end{pmatrix} \begin{pmatrix} L_2 & L' & L_t \\ -M_2 & M_s & M_t \end{pmatrix}. \quad (\text{A23})$$

Defining  $G_1$  by

$$\begin{aligned}
G_1(L, L', L_s, L_t, L_2, M_2) = & (-1)^{L+L'} \frac{(4\pi)^2}{2(2L_s + 1)^2} (L, L')^{-1/2} \sum_{M_s M_t} K_{L_s L}^{-M_s} K_{L_s L'}^{-M_s} \\
& \times \begin{pmatrix} L_2 & L & L_t \\ -M_2 & M_s & M_t \end{pmatrix} \begin{pmatrix} L_2 & L' & L_t \\ -M_2 & M_s & M_t \end{pmatrix}, \quad (\text{A24})
\end{aligned}$$

we have

$$\begin{aligned}
B_1 = & \sum_{LL'L_s L_t} \frac{1}{R^{2L_s+L+L'+2}} G_1(L, L', L_s, L_t, L_2, M_2) |\langle \Psi_a(0; \mathbf{r}) | \sum_i r_i^{L_s} Y_{L_s}(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle|^2 \\
& \times \langle \Psi_b(L_2; \rho) | \sum_j \rho_j^L Y_L(\hat{\rho}_j) | \omega(L_t; \rho) \rangle \langle \Psi_b(L_2; \rho) | \sum_j \rho_j^{L'} Y_{L'}(\hat{\rho}_j) | \omega(L_t; \rho) \rangle. \quad (\text{A25})
\end{aligned}$$

Consider the leading term of  $R^{-6}$ . The only choice is  $L_s = 1$ ,  $L = 1$ , and  $L' = 1$ . If another atom is in  $L_2 = 1$  state, then  $L_t = 0, 1$ , and  $2$ . For this case,

$$\begin{aligned}
B_1 = & \frac{1}{R^6} |\langle \Psi_a(0; \mathbf{r}) | \sum_i r_i Y_1(\hat{\mathbf{r}}_i) | \chi(1; \mathbf{r}) \rangle|^2 \\
& \times \sum_\lambda G_1(1, 1, 1, \lambda, 1, M_2) |\langle \Psi_b(1; \rho) | \sum_j \rho_j Y_1(\hat{\rho}_j) | \omega(\lambda; \rho) \rangle|^2. \quad (\text{A26})
\end{aligned}$$

Similarly, for  $B_2$  with  $L_1 = 0$ , we have

$$\begin{aligned}
B_2 = & \sum_{ll'L_sL_t} \frac{1}{R^{2L_t+l+l'+2}} G_2(l, l', L_t, L_s, L_2, M_2) |\langle \Psi_a(0; \rho) | \sum_j \rho_j^{L_t} Y_{L_t}(\hat{\rho}_j) | \omega(L_t; \rho) \rangle|^2 \\
& \times \langle \Psi_b(L_2; \mathbf{r}) | \sum_i r_i^L Y_L(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle \langle \Psi_b(L_2; \mathbf{r}) | \sum_i r_i^{l'} Y_{l'}(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle
\end{aligned} \quad (\text{A27})$$

with

$$\begin{aligned}
G_2(l, l', L_t, L_s, L_2, M_2) = & \frac{(4\pi)^2}{2(2L_t+1)^2} (l, l')^{-1/2} \sum_{M_s M_t} K_{lL_t}^{M_t} K_{l'L_t}^{M_t} \\
& \times \begin{pmatrix} L_2 & l & L_s \\ -M_2 & M_t & M_s \end{pmatrix} \begin{pmatrix} L_2 & l' & L_s \\ -M_2 & M_t & M_s \end{pmatrix}.
\end{aligned} \quad (\text{A28})$$

For  $R^{-6}$ ,  $L_t = 1$ ,  $l = 1$ ,  $l' = 1$ . Thus, for the case of  $L_2 = 1$ ,  $B_2$  becomes

$$\begin{aligned}
B_2 = & \frac{1}{R^6} |\langle \Psi_a(0; \rho) | \sum_j \rho_j Y_1(\hat{\rho}_j) | \omega(1; \rho) \rangle|^2 \\
& \times \sum_{\lambda} G_2(1, 1, 1, \lambda, 1, M_2) |\langle \Psi_b(1; \mathbf{r}) | \sum_i r_i Y_1(\hat{\mathbf{r}}_i) | \chi(\lambda; \mathbf{r}) \rangle|^2.
\end{aligned} \quad (\text{A29})$$

Finally, for  $B_3$  with  $L_1 = 0$ , we have

$$\begin{aligned}
B_3 = & \sum_{Ll'L_sL_t} \frac{1}{R^{L_s+L_t+L+l'+2}} G_3(L, l', L_s, L_t, L_2, M_2) \\
& \times \langle \Psi_a(0; \mathbf{r}) | \sum_i r_i^{L_s} Y_{L_s}(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle \langle \Psi_a(0; \rho) | \sum_j \rho_j^{L_t} Y_{L_t}(\hat{\rho}_j) | \omega(L_t; \rho) \rangle \\
& \times \langle \Psi_b(L_2; \rho) | \sum_j \rho_j^L Y_L(\hat{\rho}_j) | \omega(L_t; \rho) \rangle \langle \Psi_b(L_2; \mathbf{r}) | \sum_i r_i^{l'} Y_{l'}(\hat{\mathbf{r}}_i) | \chi(L_s; \mathbf{r}) \rangle,
\end{aligned} \quad (\text{A30})$$

with

$$\begin{aligned}
G_3(L, l', L_s, L_t, L_2, M_2) = & (-1)^{L+L_s} \frac{(4\pi)^2}{(2L_s+1)(2L_t+1)} (L, l')^{-1/2} \sum_{M_s M_t} (-1)^{M_s+M_t} K_{L_s L}^{-M_s} K_{l' L_t}^{M_t} \\
& \times \begin{pmatrix} L_2 & L & L_t \\ -M_2 & M_s & M_t \end{pmatrix} \begin{pmatrix} L_2 & l' & L_s \\ -M_2 & M_t & M_s \end{pmatrix}.
\end{aligned} \quad (\text{A31})$$

The only term which contributes  $R^{-6}$  is the one with  $L_s = 1$ ,  $L_t = 1$ ,  $l' = 1$ , and  $L = 1$ . For the case of  $L_2 = 1$ , one obtains

$$\begin{aligned}
B_3 = & \frac{1}{R^6} G_3(1, 1, 1, 1, 1, M_2) \\
& \times \langle \Psi_a(0; \mathbf{r}) | \sum_i r_i Y_1(\hat{\mathbf{r}}_i) | \chi(1; \mathbf{r}) \rangle \langle \Psi_a(0; \rho) | \sum_j \rho_j Y_1(\hat{\rho}_j) | \omega(1; \rho) \rangle \\
& \times \langle \Psi_b(1; \rho) | \sum_j \rho_j Y_1(\hat{\rho}_j) | \omega(1; \rho) \rangle \langle \Psi_b(1; \mathbf{r}) | \sum_i r_i Y_1(\hat{\mathbf{r}}_i) | \chi(1; \mathbf{r}) \rangle.
\end{aligned} \quad (\text{A32})$$

For the  $S$  state  $\Psi_a(0; \mathbf{r})$ , the parity is  $+1$ , and for the  $P$  state  $\Psi_b(1; \mathbf{r})$ , the parity is  $-1$ . Since these two states cannot be connected simultaneously to a third parity eigenstate by a dipole operator,  $B_3$  is therefore zero.

For two like atoms the spectra  $\{\chi(LM; \mathbf{r})\}$  and  $\{\omega(LM; \rho)\}$  are identical and  $B_1$  and  $B_2$  can be combined. The final expression for the second-order energy correction to the  $\text{Li}(S)\text{-Li}(P)$  system is

$$V^{(2)} = -\frac{C_6^{M_2}}{R^6}, \quad (\text{A33})$$

where

$$C_6^{M_2} = \sum_{st} \frac{\Omega_{st}}{E_{st}^{(0)} - E^{(0)}} \quad (\text{A34})$$

with

$$\begin{aligned} \Omega_{st} = & |\langle \Psi_a(0; \mathbf{r}) | \sum_i r_i Y_1(\hat{\mathbf{r}}_i) | \chi(1; \mathbf{r}) \rangle|^2 \\ & \times \sum_{\lambda} G(1, 1, 1, \lambda, 1, M_2) |\langle \Psi_b(1; \rho) | \sum_j \rho_j Y_1(\hat{\rho}_j) | \omega(\lambda; \rho) \rangle|^2. \end{aligned} \quad (\text{A35})$$

In (A35),  $G$  is defined by

$$G(1, 1, 1, \lambda, 1, M_2) = G_1(1, 1, 1, \lambda, 1, M_2) + G_2(1, 1, 1, \lambda, 1, M_2). \quad (\text{A36})$$

It is easy to see that

$$G_1(1, 1, 1, \lambda, 1, M_2) = G_2(1, 1, 1, \lambda, 1, M_2). \quad (\text{A37})$$

The algebraic coefficients  $G(1, 1, 1, \lambda, 1, M_2)$  are listed in Table I.

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# TABLES

TABLE I. The algebraic coefficients  $G(1, 1, 1, \lambda, 1, M_2)$ .

	$\lambda = 0$	$\lambda = 1$	$\lambda = 2$
$M_2 = 0$	$\frac{64}{81}\pi^2$	$\frac{16}{81}\pi^2$	$\frac{176}{405}\pi^2$
$M_2 = \pm 1$	$\frac{16}{81}\pi^2$	$\frac{40}{81}\pi^2$	$\frac{152}{405}\pi^2$

TABLE II. Values of the static polarizabilities  $\alpha_1(0)$ ,  $\alpha_2(0)$ , and  $\alpha_3(0)$  for the ground state H, He, and Li atoms.

System	$\alpha_1(0)$	$\alpha_2(0)$	$\alpha_3(0)$
H	4.5	15	131.25
He	1.383 192 174 40(5)	2.445 083 101(2)	10.620 328 6(2)
Li	164.111(2)	1 423.266(5)	39 650.49(8)

TABLE III. Comparison of static polarizabilities  $\alpha_1(0)$ ,  $\alpha_2(0)$ , and  $\alpha_3(0)$  for He( $1^1S$ ).

Author (year)	Reference	$\alpha_1(0)$	$\alpha_2(0)$	$\alpha_3(0)$
Luyckx <i>et al.</i> (77)	[17]	1.379	2.430	10.48
Thakkar (81)	[18]	1.383 12	2.443 44	10.614 4
Bishop and Pipin (93)	[7]	1.383 192	2.445 083	10.620 360
Caffarel <i>et al.</i> (93)	[19]	1.382 7	2.406 6	10.36
Jamieson <i>et al.</i> (95)	[9]	1.383 192		
Chen (95)	[20]	1.383 32		
Chen and Chung (96)	[11]	1.383 27	2.445 66	10.625 2
This work		1.383 192 174 40(5)	2.445 083 101(2)	10.620 328 6(2)

TABLE IV. Comparison of static polarizabilities  $\alpha_1(0)$ ,  $\alpha_2(0)$ , and  $\alpha_3(0)$  for  $\text{Li}(2^2S)$ .

Author (year)	Reference	$\alpha_1(0)$	$\alpha_2(0)$	$\alpha_3(0)$
Maeder and Kutzelnigg (79)	[23]	164.3	1 383	36 795
Muszyńska <i>et al.</i> (82)	[24]	163.8		
Pipin and Woźnicki (83)	[25]	163.9		
Pouchan and Bishop (84)	[26]	164(2)		
Müller <i>et al.</i> (84)	[27]	163.7		
Knowles and Meath (86)	[28]	165.8	1 486	36 495
Maroulis and Thakkar (89)	[29]	164.5	1 428	
Pipin and Bishop (92)	[22]	164.1	1 423	
Ponomarenko and Shestakov (93)	[30]	165.2		
Marinescu <i>et al.</i> (94)	[8]		1 424	39 688
Wang and Chung (94)	[31]	164.08		
Mérawa <i>et al.</i> (94)	[32]	164.8	1 430	
Kassimi and Thakkar (94)	[33]	164.2(1)		
Laughlin (95)	[34]	163.91		
This work		164.111(2)	1 423.266(5)	39 650.49(8)
Experiment (74)	[35]	164.0(3.4)		

TABLE V. Convergence of  $\text{Li}(2^2S)$   $\alpha_1(0)$  and  $\text{Li}(2^2S)\text{-Li}(2^2S)$   $C_6$  in length and velocity forms.

No. of terms	$\alpha_1(0)$ (length)	$\alpha_1(0)$ (velocity)	$C_6$ (length)	$C_6$ (velocity)
56	164.002	165.218	1 389.76	1 409.91
139	164.048	164.201	1 391.21	1 393.56
307	164.082	164.131	1 392.37	1 393.08
623	164.095	164.107	1 392.80	1 392.92
1175	164.105	164.108	1 393.17	1 393.17
1846	164.107	164.108	1 393.23	1 393.21

TABLE VI. Values of  $C_6$ ,  $C_8$ , and  $C_{10}$  for two ground state atoms.

System	$C_6$	$C_8$	$C_{10}$
H-H	6.499 026 705 405 839 313 13	124.399 083 583 622 343 609 59	3 285.828 414 967 421 697 872 5
He-He	1.460 977 837 68(5)	14.117 857 340(5)	183.691 070 5(7)
Li-Li	1 393.39(16)	83 425.8(4.2)	$73\,721(1) \times 10^2$
H-He	2.821 343 915 28(6)	41.836 376 162(8)	871.540 471(1)
He-Li	22.507(1)	1 083.16(5)	72 602.1(1)
Li-H	66.536(5)	3 279.99(2)	223 016.6(5)

TABLE VII. Comparison of  $C_6$ ,  $C_8$ , and  $C_{10}$  for the He( $1^1S$ )-He( $1^1S$ ) system.

Author (year)	Reference	$C_6$	$C_8$	$C_{10}$
Luyckx <i>et al.</i> (77)	[17]	1.458	14.06	182.16
Glover and Weinhold (77)	[37]	1.459 7(55)		
Margoliash and Meath (78)	[36]	1.458		
Bartolotti (80)	[38]	1.463 8	14.131	183.47
Thakkar (81)	[18]	1.460 82	14.111 8	183.600
R��rat <i>et al.</i> (93)	[39]	1.459 3	13.883	
Bishop and Pipin (93)	[7]	1.460 977 8	14.117 855	183.691 25
Jamieson <i>et al.</i> (95)	[9]	1.460 978		
Chen (95)	[40]	1.461 1	14.120	183.74
Chen and Chung (96)	[11]	1.461 06	14.120 8	183.765
This work		1.460 977 837 68(5)	14.117 857 340(5)	183.691 070 5(7)

TABLE VIII. Comparison of  $C_6$ ,  $C_8$ , and  $C_{10}$  for the Li( $2^2S$ )-Li( $2^2S$ ) system.

Author (year)	Reference	$10^{-3}C_6$	$10^{-4}C_8$	$10^{-6}C_{10}$
Stacey and Dalgarno (68)	[41]	1.391		
Manakov and Ovsinnikov (77)	[42]	1.360		
Margoliash and Meath (78)	[36]	1.387		
Maeder and Kutzelnigg (79)	[23]	1.389	8.089	6.901
M��ller <i>et al.</i> (84)	[27]	1.386		
Bussery and Aubert-Fr��con (85)	[43]	1.383	7.578 3	4.816 675
Marinescu <i>et al.</i> (94)	[8]	1.388	8.324	7.365
M��rawa <i>et al.</i> (94)	[32]	1.407 8	8.431 65	
This work		1.393 39(16)	8.342 58(42)	7.372 1(1)

TABLE IX. Values of the triple-dipole constants  $\nu_{abc}$  for the three ground state atoms H, He, and Li.

System	$C_6$ (This work)	$C_6$ (Ref. [41])
H-H-H	21.642 464 510 635 978 338 11	
He-H-H	8.102 240 874 3(2)	
He-He-H	3.268 064 896 1(1)	
He-He-He	1.479 558 606 3(1)	
Li-H-H	275.979(7)	276
Li-He-H	89.830(5)	89.6
Li-He-He	29.824(5)	29.6
Li-Li-H	6 133.5(5)	$6.12 \times 10^3$
Li-Li-He	1 917.27(5)	$1.91 \times 10^3$
Li-Li-Li	170 595(6)	$1.69 \times 10^5$

TABLE X. Values of  $C_3$  and  $C_6$  for the interaction between  $\text{Li}(2^2S)$  and  $\text{Li}(2^2P)$ .

$M_2$	$\beta$	$C_3$	$C_6$
0	1	11.000 226(15)	2 075.05(5)
0	-1	-11.000 226(15)	2 075.05(5)
$\pm 1$	1	-5.500 113 3(74)	1 406.08(5)
$\pm 1$	-1	5.500 113 3(74)	1 406.08(5)

TABLE XI. Comparison of  $C_6$  for the  $\text{Li}(2^2S)\text{-Li}(2^2P)$  system.

Author (year)	Reference	$C_6(M_2 = 0)$	$C_6(M_2 = \pm 1)$
Konowalov and Fish (83)	[44]	2 100(50)	1 750(100)
Vigné-Maeder (84)	[45]	2 025	1 374
Bussery and Aubert-Frécon (85)	[43]	1 927	1 301
Marinescu and Dalgarno (95)	[10]	2 066	1 401
This work		2 075.05(5)	1 406.08(5)